Fractal and compositional analysis of soil aggregation

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A soil aggregate is made of closely packed sand, silt, clay, and organic particles building up soil structure. Soil aggregation is a soil quality index integrating the chemical, physical, and biological processes involved in the genesis of soil structure and tilth. Aggregate size distribution is determined by sieving a fixed amount of soil mass under mechanical stress and is commonly synthesized by the mean weight diameter (MWD) and fractal dimensions such as the fragmentation fractal dimensions (D_f). A fractal is a rough object that can be broken down into a number of reduced-size copies of the original object. Equations have been developed to compute bounded and unbounded scaling factors as measures of fractal dimensions based on assumptions about average diameter, bulk density, shape and probability of failure of sieved particles. The log-log relationship between particle diameter and cumulative number or mass of aggregates or soil particles above a given diameter often shows more or less uniform fractal patterns. Multi-fractal (slopes showing several D_f values ≤ 3) and non fractal patterns or incomplete fragmentation ($D_f < 2 \text{ or } > 3$) have been reported. Scaling factors are curve-fitting parameters that are very sensitive to the choice of the fractal domain about breakpoints. Compositional data analysis using sequential binary partitions for isometric log ratio (ilr) coordinates with orthonormal basis provides a novel approach that avoids the assumptions and dimensional constraints of fractal analysis. Our objective was to compare MWD, fractal scaling factors and ilr coordinates using published data. In the first dataset, MWD was found to be biased by excessively high weight being given to the largest aggregate-size. Eight ilr coordinates contrasting micro- vs. macro-aggregates were related to fragmentation fractal dimensions, most of which were below 2 or above 3, a theoretical impossibility for geometric fractals. The critical ilr value separating scaling factors ≤ 3 and > 3 was close to zero. In a second dataset, the Aitchison distance computed across ilr coordinates proved to be a useful measure of the degree of soil aggregation, agradation or degradation against a reference composition such as that of primary particles, bare fallow or permanent grass. The individual contributions of ilr coordinates to the Aitchison distance can be interpreted in terms of sign and amplitude and be related to soil properties and processes mediated by soil aggregation.

1. Introduction

A soil aggregate is an assemblage of closely packed sand, silt, clay, and organic particles (Cambardella, 2006). Soil aggregation is a buildup process from primary particles to micro-aggregates (0.020 to 0.250 mm) and macro-aggregates (> 0.250 mm) (Tisdall and Oades, 1982). Soil aggregation is quantified by the distribution of sieve-size fractions of soil aggregates (Angers et al., 2008; Larney, 2008). The sieve-size fractions are synthesized by indexes such as mean weight diameter (MWD) (Van Bavel, 1949) and fractal dimensions (Rieu and Sposito, 1991a).

The *MWD* is a measure of soil aggregation computed from a few broad sieve-size fractions that capture a small part of soil structure complexity. However, information is lost after integrating aggregate-size fractions into *MWD* biased towards the largest sieve-size fractions (Cambardella, 2006; Caruso et al., 2011). As a result, soil ecologists still rely on individual sieve-size categories to describe aggregate-size distribution (Caruso et al., 2011) in order to provide higher dimensionality and finer-scale interpretation to the data. The fractal model is a log-distribution of sieve-size fractions that describes the clustering, fragmentation and fragility of geological materials (Turcotte, 1986, 1989). Fractals are assumed to be scale-invariant (Anderson et al., 1998) within a given domain. Surface fractals are objects with a fractal boundary or perimeter and a compact bulk density like a quartz particle (Anderson et al., 1998). The surface fractal dimension (D_s) is computed from the slope of the relationship between cumulative number of particles and particle size (Mandelbrot, 1983) assuming constant bulk density. Since mass fractals like soil aggregates are porous objects that have non uniform but self-similar or self-affine distribution of internal mass (i.e. bulk density decreases as aggregate size increases), mass fractal dimension (D_m) is computed from the relationship between bulk density and particle size (Anderson et al., 1998).

Fragmentation fractals are objects fragmented according to the distribution of joints and preexisting planes of weakness where the point of disjuncture is the breakpoint between two contrasting adjacent slopes (Rieu and Sposito, 1991a,b). Those fractals based on particle numbers and sizes appeared to be appropriate to model the soil aggregation building process. The slopes of data distribution patterns separated by breakpoints are measures of scaling factors (Rieu and Sposito, 1991b). Since micro- (≤ 0.250 mm) and macro-(> 0.250 mm) aggregates must have distinct behavior in soil processes (Tisdall and Oades, 1982), the point of disjuncture should be about 0.250 mm with no overlap between the two separate classes of aggregates. Fragmentation fractals are measured like surface fractals, but unlike the latter, they take into account the bulk density of particles. The fragmentation dimension (D_f) of a surface soil fractal object must be between 2 and 3. Both multi-fractal (slopes showing several D_f between 2 and 3) and non fractal ($D_f < 2$ or > 3) patterns have been reported since fractal analysis relies on optimistic assumptions about average diameter, bulk density, shape and probability of failure of soil aggregates (Crawford et al., 1993a; Caruso et al., 2011). As a result, fractal dimensions may exceed 3, a theoretical impossibility for geometric fractal objects (Rieu and Perrier 1997). The distance between two soil aggregation states as computed by fragmentation fractal analysis of particle numbers may thus be misleading. A novel approach is needed.

Techniques of compositional data analysis can be implemented to integrate aggregate-size distribution into synthetic indexes that retain fine-scale information. Sieve-size fractions are compositional since they add up to 100%. There is at least one redundant fraction producing spurious correlations and resonance in the simplex. The trivial case is a 2-compositional system where the correlation coefficient between changing components is exactly minus one since any change in one component affects the proportion of the other by exactly the same value (Thomas and Aitchison, 2006). Since uncorrelated proportions are not necessarily independent due to redundancy, correlations between proportions are difficult to interpret in any meaningful way (Butler et al., 2005). In addition, compositional data have non-normal distribution by definition since they must stay between 0 and 100% rather than being randomly distributed in the real space between -∞ and +∞. The Gaussian normal law should not be applied to the distribution of raw compositions because it is impossible to have negative fractions or proportions about confidence intervals (Diaz-Zorita et al., 2002). As a result, statistical analyses based on the normality assumption such as regression, univariate, and multivariate analyses can often lead to misleading inferences (Butler et al., 2005). Log

ratios that takes any real value can project the compositional into the real space where Gaussian laws can be applied (Aitchison, 1986). Using ad hoc sequential binary partitions of *D* fractions with orthonormal basis, isometric log ratio (*ilr*) coordinates (Egozcue and Pawlowsky-Glahn, 2005) can describe the process of soil aggregation or fragmentation in *D-1* dimensions with no loss of information. The log-log relationship underlying fractal dimensions can be partitioned into several sub-domains of higher dimensionality using *ilr* coordinates. The Aitchison distance is a synthetic index of soil aggregation computed across *ilr* coordinates selected to test a hypothesis.

The objective of this paper is to present some drawbacks of *MWD* and fractal dimensions and introduce compositional indexes of soil aggregation. In case studies, we compare *MWD*, *ilr* coordinates and fragmentation fractal dimensions and we compute the Aitchison distance as measure of soil aggregation and agradation. To our best knowledge, this paper is the first attempt comparing compositional and fractal analysis in soil science.

2. Theory

2.1. Overview

Mean weight diameter (*MWD*), fragmentation fractal dimension (D_f), and *ilr* coordinates are three different indexes that can synthesize the distribution of soil particles. Data required for computing these indexes are presented in Table 1.

Mean sieve diameter	Weight	Aggregate $W \times d$	Particle number	Fragmentation fractal data	Data for log contrast
d_1	W_1	$d_1 W_1$	$N_1 = \dfrac{W_1}{d_1^3 c \rho_1}$	$\mathrm{Ln}(N_1)$	$\mathrm{Ln}(W_1)$
d_2	W_2	$d_2 W_2$	$N_2 = \dfrac{W_2}{d_2^3 c \rho_2}$	$\mathrm{Ln}(N_1 + N_2)$	$\mathrm{Ln}(W_2)$
d_3	W_3	$d_3 W_3$	$N_3 = \dfrac{W_3}{d_3^3 c \rho_3}$	$\mathrm{Ln}(N_1 + N_2 + N_3)$	$\mathrm{Ln}(W_3)$
Synthetic index		*MWD*		D_f	$\mathcal{A}$

Table 1. Data required to compute mean weight diameter (*MWD*), fractal dimension (D_f), and *ilr* coordinate across three sieve sizes. Symbols: diameter (d), weight (W) of aggregate or total soil (primary particles and aggregates), shape coefficient (c), bulk density (ρ), number (N), and Aitchison distance ($\mathcal{A}$).

The average particle size within a size class has been defined as the diameter of a hypothetical particle representing total mass of particles irregular in shape and non-uniform in size (Green, 1923). The arithmetic mean between two sieve sizes (d_i) is an arbitrary measure of average particle diameter used to compute *MWD* and D_f,. The curvilinear relationships between mass fractions and sieve size tend to overestimate mean aggregate size (Diaz-Zorita et al., 2002). Assuming a discrete distribution of aggregates or particles rather than a continuum, the value of D_f is strongly dependent on the choice of d_i because d_i is raised to the power 3 (Anderson et al., 1998).

Whilst a fractal object undergoing complete fragmentation has power-law number- (Rieu and Sposito, 1991b) or mass fraction- (Tyler and Wheatcraft, 1992) size distribution functions, such functions do not necessarily imply fractal behavior (Crawford et al., 1993a). Kosak et al. (1996) considered the estimated fractal dimension merely as a curve fitting parameter to the logarithmic probability function. Although based on weak assumptions, the fragmentation fractal dimensions derived from scaling factors are often related to soil

functions (Crawford et al., 1993a,b; Anderson et al., 1998; Young and Crawford, 2004; Caruso et al., 2011).

The fractal cumulative function requires that particle numbers be amalgamated below a given size class while the compositional approach is based on particle numbers or mass in each size class. A discussion on the conceptual differences between compositional and fractal geometry is beyond the scope of this paper.

2.2 Mean weight diameter (*MWD*)

The *MWD* is computed across *D* sieve sizes as follows (Larney, 2008):

$$MWD = \sum_{i=1}^{D} \bar{x}_i w_i , \tag{1}$$

where $\bar{x}_i$ is the diameter for the ith fraction and w_i is the weight fraction retained on the ith sieve. Mean aggregate size is overestimated due to higher weight being attributed to larger particles and smaller weight given to smaller particles (Fig. 1). However, Eq. 1 avoids counting aggregate particles that would necessitate measuring aggregate bulk density.
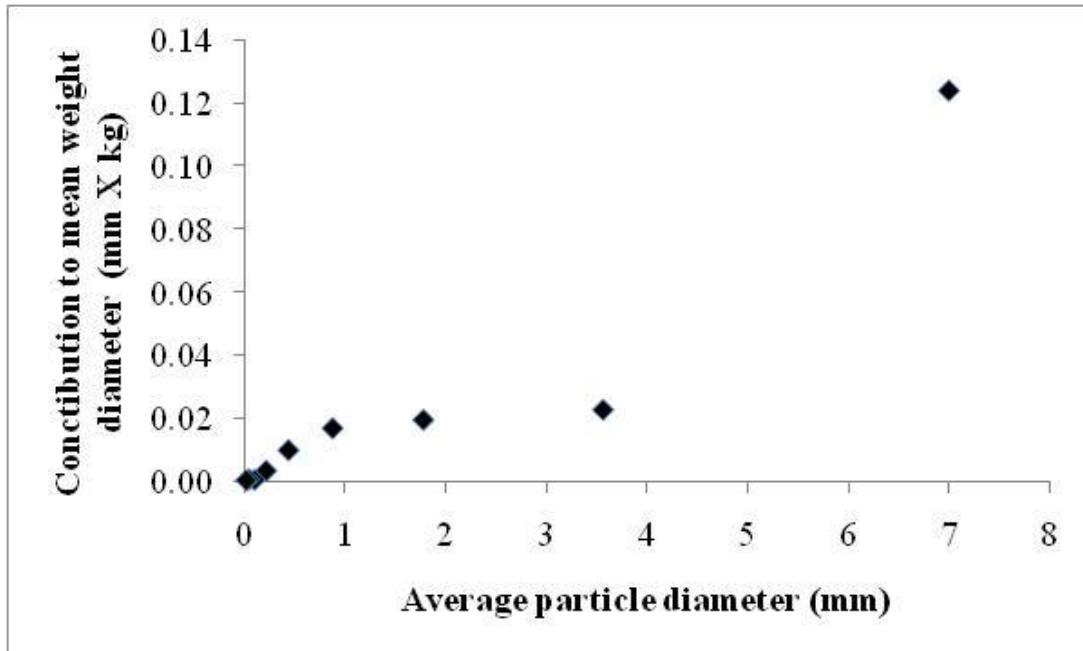

Figure 1. Relationship between particle diameter and mean weight diameter using the Wittmus and Mazurak (1958) data.

Based on an average particle diameter and sieve-size weight only, *MWD* has not been related to the theory of aggregation from primary particles to micro- and macro-aggregates.

2.3. Fragmentation fractal dimension

The fragmentation fractal dimension D_f is computed as follows (Rieu and Sposito, 1991b):

$$N(d_k) = \sum_{i=0}^{k} N(d_i) = \alpha d_k^{-D_f} \tag{2}$$

where $N(d_k)$ is the cumulative number of particles with diameter $\leq d_k$, $N(d_i)$ is the number of particles in the ith size fraction and α is a proportionality parameter; D_f is a scaling factor interpreted as a fragmentation fractal dimension and computed from the log-log relationship between $N(d_k)$ and d_k. The number of particles $N(d_i)$ in the ith size fraction is computed

from total mass of aggregate $M(d_i)$ of bulk density ρ_i and shape coefficient c_i in the ith size class as follows (Hatch, 1933; Perfect et al., 1992; Kozak et al., 1996):

$$N(d_i) = M(i)/(d_i^3 c_i \rho_i), \tag{3}$$

where $M(i)$ is the mass of size class *i*. In Eq. 3, bulk and particle density values are measured or assumed to be independent of scale. Techniques for measuring ρ_i across a large range of aggregate-size classes are imprecise (Logsdon, 1995). Soil particle density vary within a narrow range of 2.60 to 2.75 g cm^{-3} in most mineral soils since quartz, feldspar, micas, and colloidal silicates having densities within this range make up the major portion of mineral soils (Brady, 1990). Aggregates are generally assumed to be cubic and primary particles to be spherical (Anderson et al., 1998). The shape coefficient is a surface to volume relationship equal to 6 for the diameter of a sphere and the edge of a cube (Green, 1923).

The mechanical stress imposed by sieving methods may bias particle counts required to compute fractal dimensions (Diaz-Zorita et al., 2002). If fragments bear no resemblance with the original arrangement the fractal dimension may exceed 3 (Turcotte, 1992; Anderson et al., 1995). Since larger aggregates are more likely to break than smaller ones at the same level of applied stress (Freudenthal, 1968), fractal dimensions may reach $3 + r$ where *r* determines the extent of scale dependency of the probability of failure of the initiator (Perfect et al., 1993a,b).

To avoid fractal dimensions exceeding 3, Tyler and Wheatcraft (1992) developed an equation to compute surface fractals from mass fractions only, rearranged as follows by Caruso et al., (2011):

$$\log\bigl(M(r^* < R)\bigr) = \log k_2 + k_1 \log(r^*) \tag{4}$$

where *M* is cumulative mass, r^* is a sieve size, *R* is the largest sieve size and k_2 and k_1 are equation parameters. Setting $k_1 = D_f - 3$ avoids deriving surface fractal dimensions exceeding 3. The D_f is thus bounded to 3 in Eq. 4 and is unbounded in Eq. 2.

Difficulties in determining average particle or aggregate diameter, bulk density, shape or probability of failure can be largely avoided using sieve-size categories and techniques of compositional data analysis.

2.4. Compositional space of soil aggregates

Considering the soil as a mixture of primary particles and aggregates of different dimensions, a composition made of *D* fractions is compositional since the sum of mass fractions is bounded to the initial total mass. A *D*-part composition $x = [x_1, x_2, \ldots, x_D]$ is described by its parts as follows:

$$x = \mathcal{C}(x_1, x_2, \ldots, x_D) = \left(\frac{x_1 \kappa}{\sum_{i=1}^{D} x_i}, \frac{x_2 \kappa}{\sum_{i=1}^{D} x_i}, \ldots, \frac{x_D \kappa}{\sum_{i=1}^{D} x_i} \right), \tag{5}$$

where $\mathcal{C}$ is the closure operator to unit κ (Aitchison, 1986). The scale of measurement must be invariant across components. For example, the compositional analyst may use $\kappa = 1$ for fractions, $\kappa = 100$ for proportions, and $\kappa = mg\ kg^{-1}$ for parts per million.

Log-ratio transformations used to project compositional data from the compositional to the real space have specific geometric characteristics (Egozcue and Pawlowsky-Glanh, 2006). The additive log ratio (*alr*) has oblique geometry restricting data representation on axes. The centered log ratio (*clr*) is measured in *D* rather than *D-1* dimensions, hence leading

to singular matrices. The isometric log-ratio technique (*ilr*) implies a sequential ad hoc ordering of *D* size fractions that can be combined into *D-1* sequential binary partitions with orthonormal bases (Egozcue and Pawlowsky-Glanh, 2005; Egozcue and Pawlowsky-Glanh, 2006). Binary partitions can be selected to represent the main processes mediating soil aggregation. The ith isometric log ratio (*ilr*) coordinate representing binary partition x_i^* is computed as a contrast between two groups of parts shown by the plus (+) and minus (−) signs, respectively, as follows (Egozcue and Pawlowsky-Glahn, 2006):

$$x_i^* = \sqrt{\frac{rs}{r+s}} \, ln \frac{g(x_+)}{g(x_-)}, \tag{6}$$

where *r* is the number of parts in the + group, *s* is the number of parts in the − group, $g(x_+)$ is the geometric mean of components in group x_+ and $g(x_-)$ is the geometric mean of components in group x_-. Soil aggregation, degradation or agradation can be measured as the Aitchison distance $\mathcal{A}$ between a given and a reference composition as follows (Egozcue and Pawlowsky-Glanh, 2006):

$$\mathcal{A}^2(x,y) = \sum_{i=1}^{D-1}(x_i^* - y_i^*)^2 \text{ and } \mathcal{A} = \sqrt{\mathcal{A}^2(x,y)}, \tag{7}$$

If the distribution of primary particles among sieve sizes is similar in x_i^* and y_i^*, the difference between x_i^* and y_i^* provides a measure of soil aggregation from primary particles. If the distribution of aggregates among sieve sizes changes from x_i^* to y_i^* as a result of a treatment over control, the difference between x_i^* and y_i^* provides a measure of soil agradation or degradation. The sign of the difference between x_i^* and y_i^* indicates in what direction soil aggregation changes and its amplitude indicates the size that change.

2.5. **Bulk density and shape coefficient as perturbations on mass**

In compositional data analysis, a perturbation is an operation whereby composition *x* changes to *X* through a perturbation vector *u* as follows (Aitchison, 1986):

$$X = \mathcal{C}(u_1 x_1, \dots, u_D x_D) \tag{8}$$

where $\mathcal{C}$ indicates closure of the vector space to the appropriate unit (in general, 100%). The inverse operation is a division (Egozcue, and Pawlowsky-Glahn, 2006).

Considering sieve sizes as categorial variables, particle diameter, bulk density and shape coefficient can be viewed as perturbations on mass or shifts in the simplex (Egozcue and Pawlowsky-Glahn, 2006). The perturbation vector thus sets apart particle properties subjected to assumptions under fractal analysis of the aggregate-size distribution. Difference in particle numbers defined by a binary partition between two sub-compositions τ and ν making up the + and− group (Eq. 6), respectively, is computed as follows:

$$\ln[N(d_\tau)] - \ln[N(d_\nu)] = ln \frac{M(d_\tau)/(d_\tau^3 c_\tau \rho_\tau)}{M(d_\nu)/(d_\nu^3 c_\nu \rho_\nu)} = \ln \frac{M(d_\tau)}{M(d_\nu)} - \left[\ln \frac{(d_\tau^3 c_\tau \rho_\tau)}{(d_\nu^3 c_\nu \rho_\nu)} \right] \tag{9}$$

where the expression in brackets is the perturbation of particle geometric properties and bulk density on particle mass. Since fractal objects are self-similar, *c* is invariant within scale limits (Anderson et al., 1998) and $c_{i\tau}$ and $c_{i\nu}$ thus cancel out. Fractal analysis showed that bulk density of aggregates decreases with aggregate size (Rieu and Sposito, 1991b; Perfect et al., 1993b) as follows:

$$\rho_i/\rho_o = (d_i/d_o)^{D_m-3} \text{ and } ln(\rho_i/\rho_o) = (D_m - 3)ln(d_i/d_o), \tag{10}$$

where D_m is mass fractal dimension, ρ_i is bulk density of aggregates in i^{th} size class, ρ_o is bulk density of aggregates in the largest size class, d_i is the diameter of particles in i^{th} size class, and d_o is the diameter of particles in the largest size class. The mass fractal dimension is computed from the slope of the log-log relationship between ρ_i and d_i. Replacing $\rho_{i\tau}$ and ρ_{iv} by their fractal expression in Eq. 10, we obtain:

$$ln(\rho_\tau/\rho_v) = (D_m - 3)ln(d_\tau/d_v) \tag{11}$$

where D_m and d_τ/d_v are constant values for a given *ilr* coordinate. Introducing Eq. 11 into Eq. 9, we obtain:

$$ln[N(d_\tau)] - ln[N(d_v)] = ln\frac{M(d_\tau)}{M(d_v)} - [D_m ln(d_\tau/d_v)] \tag{12}$$

The expression in brackets is a translation of mass in the simplex. Since particles free to move in a fully dispersed system with no cluster form a 3-*D* reactive system (Kopelman, 1988), D_m is a constant close to 3 for a dispersed soil and to the D_m values of 2.88 to 2.95 for the Chepil (1950) soils as computed by Rieu and Sposito (1991b). As a result, the difference between two *ilr* coordinates can be measured from mass log ratios only.

3. The Wittmus and Mazurak (1958) dataset

Rieu and Sposito (1991b) used Sharpsburg soil aggregate data from Wittmus and Mazurak (1958) to compute mass and fragmentation fractal dimensions across nine sieve sizes. The distribution of size weight fractions is presented in Fig. 1.
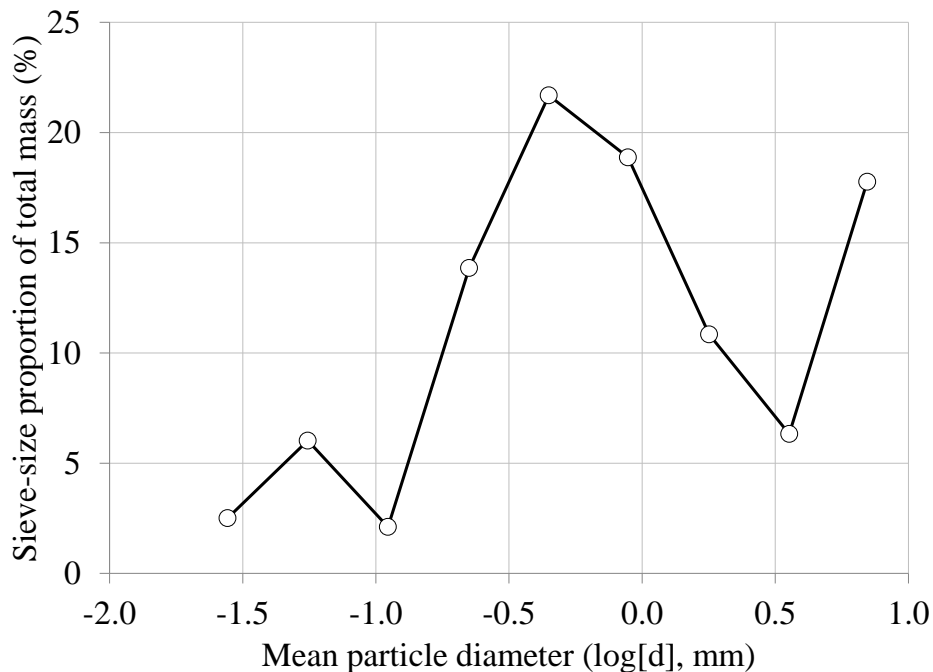

Figure 1. Distribution of size weight fractions of aggregates in a Sharpsburg soil (Wittmus and Mazurak, 1958').

The relationship between aggregate bulk density and aggregate size showed a dual pattern with an apparent point of disjuncture at 0.111 mm (Fig. 2). The choice of the

breakpoint may be arbitrary as driven by the data. A more theoretically sound choice would be 0.224 mm, i.e. near the limit between micro- and macro-aggregate at 0.250 mm.
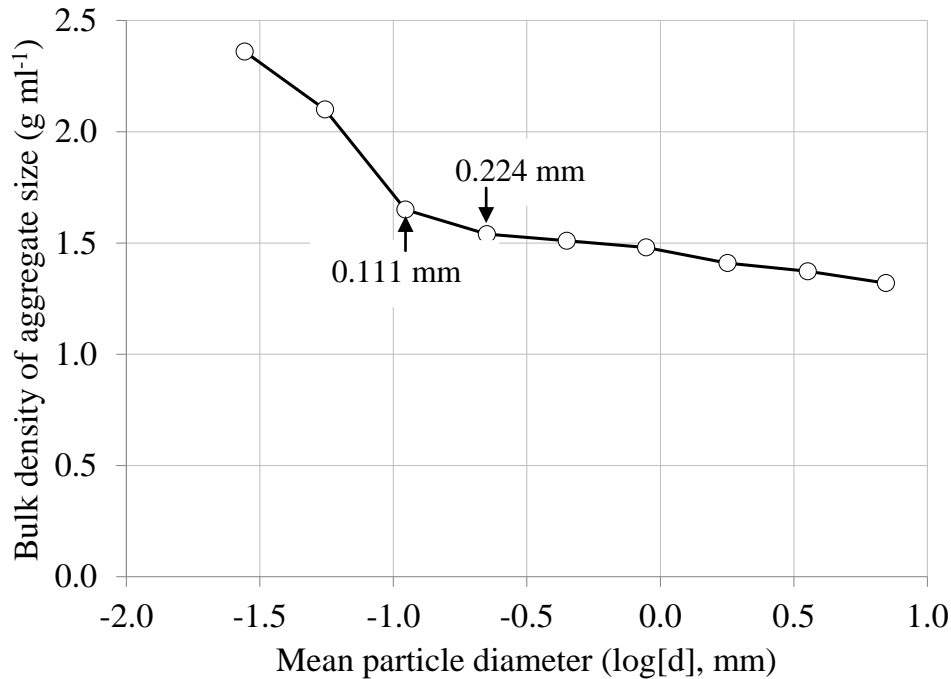

Figure 2. Distribution of bulk density of aggregate sizes in a Sharpsburg soil (Wittmus and Mazurak, 1958).

The data required to solve Eqs. 2 to 4 are presented in Table 2.

Mean sieve size mm	Soil mass kg	Bulk density Mg m^{-3}	Cumulated number of particles	Cumulated weight kg
7.005	0.0177	1.320	3.901E-05	0.0177
3.57	0.0063	1.373	1.399E-04	0.0240
1.785	0.0108	1.410	1.487E-03	0.0348
0.885	0.0188	1.480	1.981E-02	0.0536
0.446	0.0216	1.510	1.811E-01	0.0752
0.224	0.0138	1.540	9.783E-01	0.0890
0.111	0.0021	1.650	1.909E+00	0.0911
0.0555	0.0060	2.100	1.862E+01	0.0971
0.02775	0.0025	2.360	6.819E+01	0.0996

Table 2. Mean sieve diameter and computed number of particles of cubic shape and known bulk density used to compute fragmentation fractal dimensions.

There were contrasting fractal patterns between micro- and macro-aggregates using a breakpoint between 0.224 and 0.446 mm. The unbounded D_f (Eq. 2) were 2.16 and 3.17 for micro- ($\leq$ 0.224 mm) and macro- ($\geq$ 0.446 mm) aggregates, respectively (Fig. 3). Fractal dimensions were sensitive to the choice of the breakpoint. For the shared breakpoint at 0.111 mm, the unbounded D_f values were found by Rieu and Sposito (1991b) to be 2.58 for micro-aggregates ($\leq$ 0.111 mm) and 2.84 for larger aggregates ($\geq$ 0.111 mm).
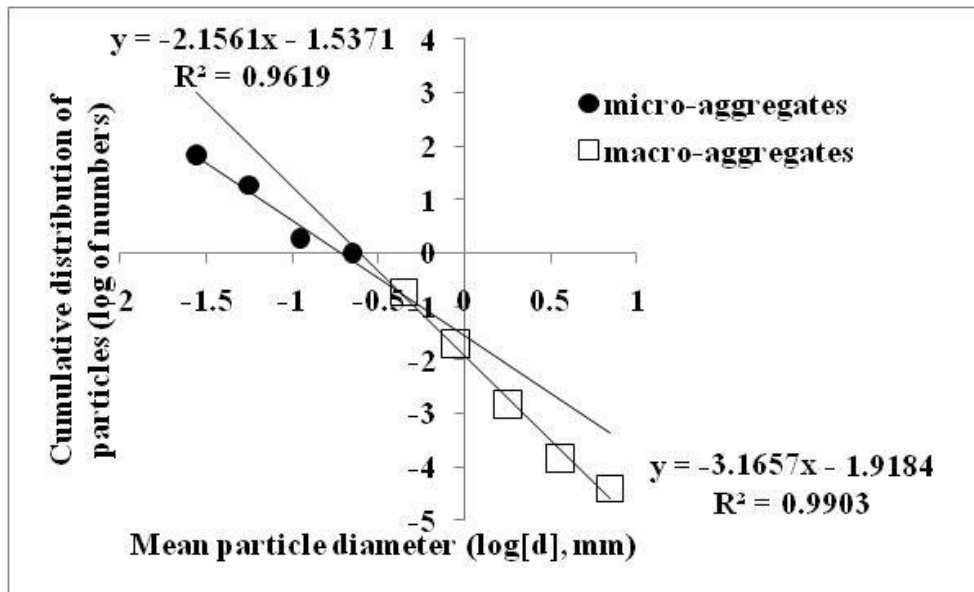
Figure 3. Unbounded fractal scaling factors for micro- and macro-aggregates in a Sharpsburg soil.

In comparison, the bounded D_f values were 1.99 and 2.74 for micro- ($\leq$ 0.224 mm) and macro-aggregates ($\geq$ 0.224 mm), respectively (Fig. 4).
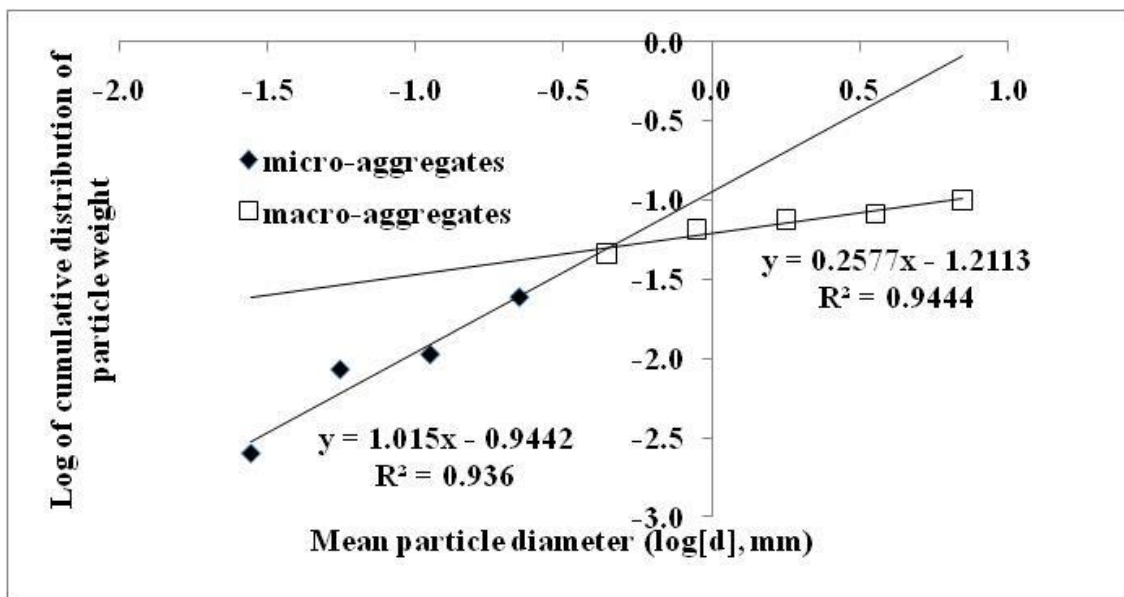

Figure 4. Bounded fractal scaling factors ($D_{f-unbounded}$ = 3 minus slope) for micro- and macro-aggregates in a Sharpsburg soil.

There was a significant correlation between bounded and unbounded D_f embedded in other *ilr* coordinates (r = 0.894, *P < 0.01*).

Sequential binary partitions were arranged to match the fractal domains of micro- and macro-aggregates. There were eight *ilr* coordinates (D-1) or compositional dimensions from nine aggregate-size fractions (Table 3). The first one (*ilr1*) is the primary partition between micro- and macro-aggregation domains based on the theory of Tisdall and Oades (1982). Since the principle of orthogonality controls the choice of binary partitions, there was no shared point of disjuncture between two fractal objects as in Rieu and Sposito (1992b). The *ilr2* was so defined as to set apart the largest aggregate-size fraction that was the common

denominator (d_o) to compute mass fractal dimension (Eq. 10). Other *ilr* coordinates were sub-partitions of the upper ones.

Ilr	Macro-aggregate fractions					Micro-aggregate fractions				r	s
	Average size (mm)										
	7.005	3.57	1.785	0.885	0.446	0.224	0.111	0.0555	0.02775		
1	1	1	1	1	1	-1	-1	-1	-1	5	4
2	1	-1	-1	-1	-1	0	0	0	0	1	4
3	0	1	1	-1	-1	0	0	0	0	2	2
4	0	1	-1	0	0	0	0	0	0	1	1
5	0	0	0	1	-1	0	0	0	0	1	1
6	0	0	0	0	0	1	1	-1	-1	2	2
7	0	0	0	0	0	1	-1	0	0	1	1
8	0	0	0	0	0	0	0	1	-1	1	1

Table 3. Sequential binary partitions of aggregate-size fractions in a Sharpsburg soil.

The *ilr* coordinates were related to their corresponding bounded and unbounded fractal dimensions for particles within the same domain. Due to the bi-fractal behaviour of Sharpsburg soil aggregation, *ilr1* was useless. The *ilr* coordinates were negative for unbounded scaling factors larger than 3 except for *ilr2* (Fig. 5) likely due to larger mass retained on the upper sieve (4.76 - 9.25 mm) than on the next one (Fig. 2).
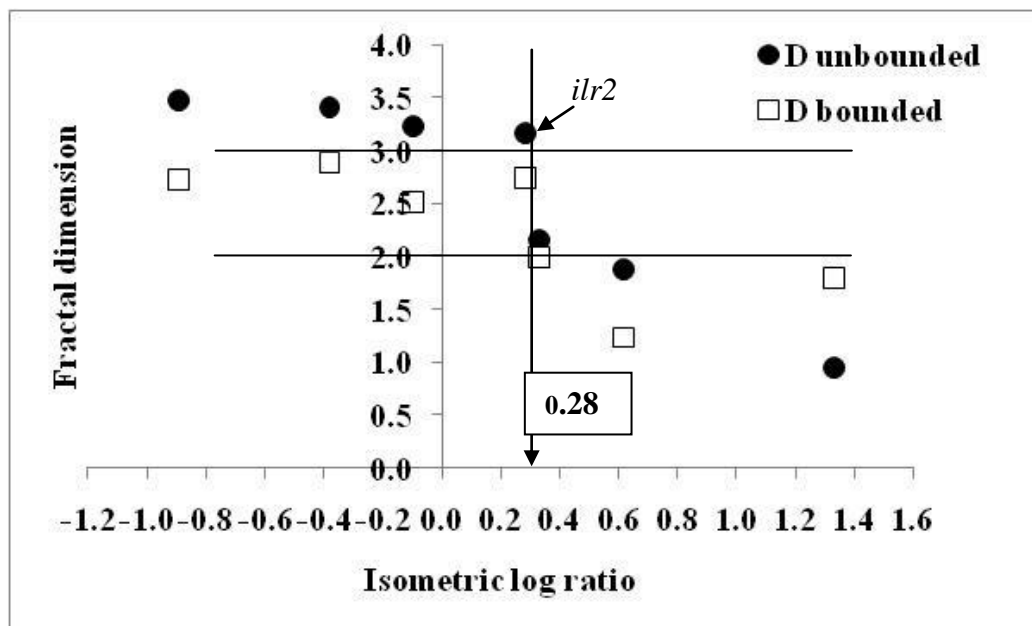

Figure 5. Relationship between *ilr* coordinates and fragmentation fractal dimensions (D_f) computed over the same domain. The D_f ranges from 2 to 3 for a soil geometrical fractal object, i.e. between the dimension of a surface and that of a volume.

The critical *ilr* value between scaling factors above and below 3 was 0.28 (Fig. 5). There were five scaling factors below 2, the minimum fractal dimension for a surface fractal, indicating that the fragmented object was not fractal or the fragmentation process was incomplete (Crawford et al., 1993a; Caruso et al., 2011). Although the critical *ilr* value was

not well defined for fractal dimensions less than 2, the range of *ilr* coordinates appeared to be narrow for fractal dimensions between 2 and 3, possibly between 0.28 and 0.33.

If fractal dimensions are merely scaling factors that are ill-defined in terms of fractal patterns (Kozack et al., 1996), *ilr* coordinates are preferable. They provide higher dimensionality with no loss of information as required by soil ecologists (Caruso et al., 2011) and are not subjected to the set of assumptions required to compute fractal dimensions likely to vary outside their geometric limits. For this dataset, the *ilr* approach generated eight dimensions compared to two dimensions for the fragmentation fractal models. Such higher dimensionality may help solving complex problems related to soil biological, chemical and physical processes mediating or driven by soil aggregation using a detailed description of soil structure.

4. The Wohlenberg et al. (2004) dataset

Wohlenberg et al. (2004) monitored changes in soil aggregate-size classes (8.00-4.76 mm; 4.76-2.00 mm; 2.00-1.00 mm; 1.00-0.21 mm; < 0.21 mm) in a Hapludalf sandy loam of southern Brazil after 7 years of bare fallow, permanent grass cover or annual crops grown in rotation. Balance coefficients to compute the degree of soil agradation for this dataset are presented in Table 4.

Ilr contrast	Aggregate-size fractions (mm)					r	s
	8.00 − 4.76	4.76 − 2.00	2.00 − 1.00	1.00 − 0.21	< 0.21	(+ signs)	(- signs)
1	1	1	1	1	-1	4	1
2	1	1	-1	-1	0	2	2
3	1	-1	0	0	0	1	1
4	0	0	1	-1	0	1	1

Table 4. Balance coefficients to compute coordinates for aggregate-size data from Wohlenberg et al. (2004).

As shown by the Aitchison distance against bare fallow, the degree of soil agradation was higher under permanent grass compared to rotation crops (Table 5) since macro-aggregates depend largely on roots and hyphae (Tisdall and Oades, 1982) that are more abundant under permanent grass.

Treatment	Aggregate-size category (mm)				
	8.00 − 4.76	4.76 − 2.00	2.00 − 1.00	1.00 − 0.21	< 0.21
	Proportion of total mass (%)				
Bare fallow	3.88	4.56	2.96	32.19	56.42
Permanent grass	96.59	2.98	0.04	0.22	0.17
Rotation crops	82.592	7.996	0.466	1.688	7.258
	ilr1	*ilr2*	*ilr3*	*ilr4*	Aitchison distance
Bare fallow	-1.946	-0.842	-0.114	-1.687	-
Permanent grass	1.793	5.198	2.460	-1.205	7.570
Rotation crops	-0.375	3.366	1.651	-0.910	4.889

Table 5. Degree of soil agradation of an Alfisol after 7 years of cropping over bare fallow.

Wohlenberg et al. (2004) provided soil texture data for sand (2.00-0.050 mm), silt (0.050-0.002 mm), and clay fractions (< 0.002 mm) for each treatment. The distribution of primary particles was reconstituted to match texture data with the distribution of aggregates

(2.00-1.00 mm; 1.00-0.21 mm; < 0.21 mm) using the Gardner (1956) log-log equation. Since some aggregate-size fractions exceeded 2 mm, the upper limit for defining soil texture, aggregate fractions exceeding 2 mm were amalgamated with the ≥ 1 mm fraction. The *ilr* coordinates to measure the degree of aggregation of primary particles were computed from the following sequential binary partitions: a contrast between larger (> 0.21 mm) and smaller aggregates (≤ 0.21 mm) and a contrast between the two categories of larger aggregates (2.00-1.00 mm and 1.00-0.21 mm). The $\mathcal{A}$ was computed following Eq. 7 as a distance between sieve-size distribution in aggregated soils and the distribution of primary particles in the same soil (Table 6).

Treatment	Particle size (mm)			Compositional metrics		
	2,00-1,00	1,00-0,21	<0,21	*ilr1*	*ilr2*	Aitchison distance
	Proportion of total mass (%)					
	Composition of primary particles					
Bare fallow	13.5	26.9	59.6	-0.931	-0.485	
Permanent grass	13.5	27.1	59.4	-0.924	-0.490	
Rotation crops	13.6	27.1	59.3	-0.922	-0.488	
	Composition of aggregates					Aggregation
Bare fallow	11.4	32.2	56.4	0.253	-0.734	0.253
Permanent grass	99.6	0.2	0.2	6.030	4.324	6.030
Rotation crops	91.1	1.7	7.3	3.576	2.820	3.576

Table 6. Degree of soil aggregation of an Alfisol after 7 years of soil treatments.

This acid (pH 5.2-6.2) Brazilian sandy Alfisol exposed for 7 years to a high precipitation (1300-1800 mm) regime (Wohlenberg et al., 2004) showed almost complete loss of structure after 7 years of bare fallow as shown by the small Aitchison distance between bare fallow and the reference composition of primary particles and the large distance between bare fallow and permanent grass and crop rotation systems. As a result, the Aitchison distance provided a useful measure of the degree of aggregation of primary particles and of soil structural improvement under different cropping systems in this structurally weak Alfisol.

5. Conclusion

The soil aggregation status is generally defined from sieve-size fractions by mean weight diameter and fractal dimensions under optimistic assumptions about aggregate diameter, bulk density, shape coefficient, and probability of failure. The *MWD* was driven by the highest weight being given to the largest aggregate size. The scaling factors used to represent fractal dimensions were often found to be outside their theoretical dimensional limits between 2 and 3 and to be very sensitive to the choice of the disjuncture point between two fractal objects.

The *ilr* coordinates using mass fractions and sequential binary partitions based on the theory of soil aggregation provide an unbiased framework for assessing the quality of soil structure. Several orthonormal dimensions can describe in more details than *MWD* and fractal dimensions many facets of soil aggregation without cumbersome assumptions on aggregate diameter, bulk density, shape, probability of failure, and geometric limits. We found that *ilr* coordinates below 0.28 were indicative of fractal dimensions exceeding 3. The high dimensionality of soil structure provided by *ilr* coordinates may reveal in more details with no loss of information the soil chemical, biological, and physical processes and functions mediating or driven by soil aggregation.

Using soil texture or bare fallow as reference compositions, the Aitchison distance, that is decomposable into *ilr* distances with direction and amplitude, is a promising measure of soil aggregation, degradation or agradation that may guide selecting the most appropriate soil and crop management techniques.

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